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LINEAR COMBINATION OF GAUSSIAN-TYPE ORBITALS
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D-D INTERACTIONS IN TITANIUM AND PALLADIUM*

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Linear combination of Gaussian-type orbitals—local-density-functional cluster studies of D-D interactions in titanium and palladium

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Linear combination of Gaussian-type orbitals (LCGTO) –local-density-functional (LDF) cluster calculations give the interaction energy of two deuterium atoms in the interstices of titanium and palladium. Octahedral and tetrahedral interstices of the face-centered-cubic (fcc) lattice are modeled by six and four metal atoms, respectively. No short equilibrium separations, compared to the gas-phase equilibrium separation, are found even when expansion of the lattice and loading with additional deuterium and metal atoms are considered. The deuterium affinities of these clusters are in accord with the experimental site preference.

I. INTRODUCTION

There is some experimental evidence for fusion accompanying the room-temperature electrochemical insertion of deuterons into titanium and palladium cathodes,^{1,2} although some of this evidence has been challenged.^{3–5} It has been hypothesized that fusion, specifically piezonuclear fusion,⁶ can result from these lattices statically squeezing pairs of deuterons together.^{2,7–9} A growing body of evidence suggests that this is not possible for the palladium deuteride system.^{10–16} For small enough D-D separations the forces pushing the two deuterons apart are, to high accuracy, the forces arising from their bare Coulomb repulsion.^{15–18} In this work we compare the interaction energy of a pair of deuterons at chemically important separations in the octahedral and tetrahedral interstices of face-centered-cubic (fcc) Pd and Ti.

To compute these interaction energies, we use the linear combination of Gaussian-type orbitals (LCGTO) –local-density-functional (LDF) method^{19–21} and a cluster of metal atoms to model these interstices. In Sec. II we describe our Gaussian basis sets and our choice of LDF's. In Sec. III we describe how we computed the interaction energies and how we constructed the clusters. Section IV describes the resultant potential-energy curves. In Sec. V we consider, for the titanium hydride system only, the effects of expanding the lattice and of loading it with deuterium. Section VI contains our conclusions.

II. BASIS SETS

In our LCGTO-LDF calculations, the Ti basis set was $15s/10p/6d$, the Pd orbital basis set was a $17s/11p/8d$ basis,²² and the D (or equivalently H) orbital basis set was a $6s$ basis.²³ The Ti basis set was the $14s/9p/5d$ basis of Wachters,²⁴ augmented with s , p , and d exponents of 0.2, 0.1, and 0.07 bohrs^{-2} , respectively. These basis sets were augmented with f polarization functions of exponent 0.5 and 1.0 bohrs^{-2} on Ti and Pd, respectively, and with p polarization functions of exponent 1.0 bohrs^{-2} on D. The f exponent for Ti is a slight improvement over the

one for Pd; such functions are rather unimportant in LCGTO-LDF calculations and for compact clusters can become numerically degenerate with lower angular-momentum basis functions.²¹ The Ti orbital basis contraction scheme was 3,5/2,3/1,3. In this notation successively higher angular momenta are separated by a slash with the first number giving the number of the (lowest-energy) atomic orbitals and the second giving the number of the (most diffuse) uncontracted Gaussians used in the cluster calculations. The Pd orbital basis contraction scheme was 4,5/3,3/1,4, and the D orbital contraction scheme was 1,4. Spherically symmetric basis sets for fitting the potential were scaled from these orbital basis sets.¹⁹ Angular variation in the potential was fit using Gaussians with exponents 0.04, 0.2, 0.6, 2.0, and 10.0 bohrs^{-2} on Ti and Pd and 1.0 bohrs^{-2} on H. The angular parts of these nonspherical fitting functions included all spherical harmonics about each center that have the two lowest (Ti and Pd) and single lowest (H) total angular momenta allowed by the symmetry of the site occupied by each atom. The calculations were nonrelativistic. Relativistic corrections for palladium will have only a minor effect on the results²⁵ and titanium has an even smaller nuclear charge.

Two LDF's were used in these calculations: $X\alpha$ (Ref. 26) (with $\alpha=0.7$), and the Perdew-Zunger (PZ) parametrization²⁷ that is based on essentially exact Monte Carlo calculations of Ceperley and Alder for the electron gas.²⁸ $X\alpha$ tends to overestimate the spin or magnetism of ground states,²⁹ while functionals that are parametrized to the correlated electron gas, like PZ, tend to overestimate binding energies.³⁰ For both Ti_6D and Ti_4D , PZ gave three unpaired spins for the ground state, while $X\alpha$ gave at least twelve. Calculations on the equivalent Pd clusters using both LDF's gave only a single unpaired spin for both ground states. Therefore we chose PZ for our titanium-containing cluster calculations and $X\alpha$ for our palladium-containing cluster calculations. To compare our binding-energy curves for titanium clusters with those for palladium, the titanium energies should be reduced by about 20%. In any single figure to follow, all curves should be scaled the same, however, and there

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would be little change in the relative positions of curves if they had been computed in the other LDF. All of the following calculations were spin restricted for even-electron systems and were spin-unrestricted (but constrained to have a single unpaired electron) for odd-electron systems.

III. CLUSTER MODELS

We chose to perform most of our calculations with nearest metal-metal distances fixed at essentially the nearest-neighbor distance of the empty lattice. For palladium this distance is 5.2 bohrs.³¹ Empty crystalline titanium has the hexagonal close-packed (hcp) structure. For this crystal the nearest-neighbor distance is 5.58 in the close-packed planes, and connecting one such plane to the next in the *c*-axis direction, the nearest-neighbor distance is 5.47 bohrs.³² For our titanium clusters we chose to use the larger of these distances, 5.58 bohrs. Clusters of such dimension are the most compact that deuterium atoms are likely to see in either lattice. Because both lattices expand upon taking up deuterium, clusters of these dimensions are most appropriate to the dilute limit. In going from pure palladium to PdD_{0.6}, the fcc lattice expands 3.5%,³¹ and Daw and Baskes predict 4% for PdD.³³ In going from hcp Ti to fcc TiD₂, the Ti-Ti nearest-neighbor distance increases by roughly 8% to 5.94 bohrs.

The effective interaction, $U_{DD}(r)$, between two deuterium atoms separated by a distance r in a cluster of n metal atoms is the total energy of a pair of deuterium atoms in the cluster minus twice the total energy of the same cluster containing a single deuterium atom at a symmetric reference position plus the total energy of the empty cluster,

$$U_{DD}(r) = E(M_n D_2; r) - 2E(M_n D) + E(M_n).$$

If this expression is negative for any r inside the cluster and the cluster adequately models the interstice, then two deuterium atoms would prefer to pair at the distance r_0 that minimizes $U_{DD}(r)$ inside the interstice rather than disperse and occupy separate interstices. We define the binding energy, $E_{DD}(r)$, in each cluster similarly, but referencing two dissociated D atoms in free space,

$$E_{DD}(r) = E(M_n D_2; r) - 2E(D) - E(M_n).$$

These two energies are related to the deuterium affinity of the reference position in the cluster, and to the extent that the cluster models the interstice, the deuterium affinity of the interstitial site,

$$W_D^{\text{site}} = -E(M_n D) + E(M_n) + E(D).$$

In Table I we give the deuterium affinity of the tetrahedral and octahedral sites, modeled using our four- and six-metal-atom clusters. For palladium, in agreement with experiment, deuterium atoms prefer the octahedral site. In the same table we also consider titanium. In its hcp crystal the only interstices are in the shape of a slightly distorted tetrahedron. Nevertheless, we computed, in the same way, the deuterium affinity of the

TABLE I. Cluster deuterium affinities.

Cluster	Affinity (eV)
Pd ₆	2.99
Pd ₄	2.93
Ti ₆	4.08
Ti ₄	4.22

tetrahedral and octahedral sites of a hypothetical fcc crystal having our chosen 5.58-bohrs nearest-neighbor distance. The ordering of our titanium cluster affinities is opposite that of our palladium cluster affinities. These calculated titanium affinities are consistent with the experimental fact that TiD does not assume a fcc structure in which all octahedral sites are occupied by a deuterium atom. Taken all together, these calculations suggest that deuterium migration in metals can be modeled well using small clusters that are allowed to change their number of metal atoms appropriately as the deuterium atom proceeds.

IV. CHEMICAL FORCES

The preferred site for deuterium in palladium is the octahedral site. To get a rather complete picture of the potentials involved for two deuterium atoms interacting through the center of the octahedral site, we performed LCGTO-LDF calculations on three different centrosymmetric Pd₆D₂ clusters. The first is D_{3d} symmetric with the deuterium atoms approaching each other along the line connecting the center of opposite faces of the octahedron formed by the six palladium atoms, i.e., along the {111} direction of the fcc lattice. The second is D_{2h} symmetric with the D-D axis along the line connecting

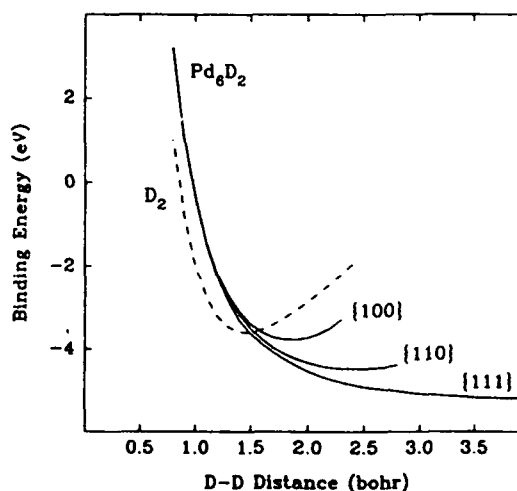


FIG. 1. The solid curves depict calculated binding-energy curves of the Pd₆D₂ cluster within the LCGTO-LDF approach for centrosymmetric arrangements of deuterium pairs along {100}, {110}, and {111} directions of the fcc lattice. The dashed line depicts the free D₂ curve, also calculated using LCGTO-LDF method. Note that the minima seen along the {100} and {110} directions are unstable.

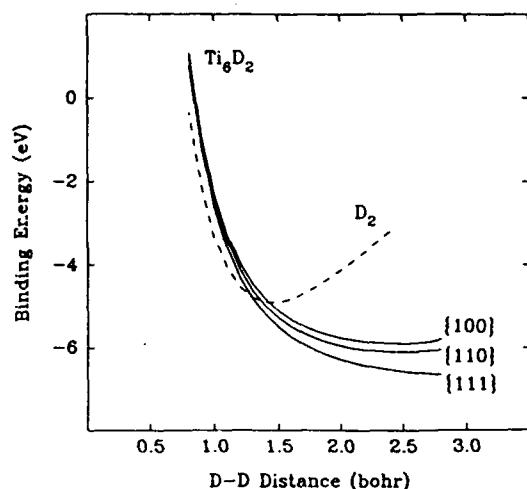


FIG. 2. Same as Fig. 1, but for titanium instead of palladium.

the centers of the nearest-neighbor Pd—Pd bonds that form opposite edges of the octahedron, i.e., along the $\{110\}$ direction of the fcc lattice. The third is D_{4h} symmetric with the D—D axis along a line connecting two second-nearest-neighbor Pd atoms at opposite vertices of the octahedron, i.e., along the $\{100\}$ direction of the fcc lattice. The binding energies of these clusters are plotted in Fig. 1. They suggest that two deuterium atoms placed into an octahedral interstice will rotate into the $\{111\}$ direction and repel at least one atom out of the interstice. This picture is supported by calculations^{10,16} using embedded-atom-method empirical potentials. Figure 2 shows that the same thing happens in the octahedral

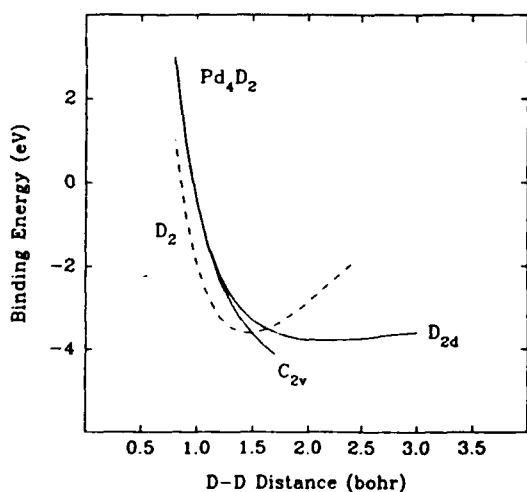


FIG. 3. LCGTO-LDF D-D binding energy curves for two directions in the tetrahedral interstice modeled by four palladium atoms (solid lines) and compared with the free D_2 curve (dashed line). The least bound curve showing a metastable minimum at 2.1 bohrs is for the D_{2d} cluster which has the D_2 axis passing through opposite nearest-neighbor Pd—Pd bonds. The C_{2v} curve is more bound, but it pushes both deuterium atoms out of the site. Both curves are discontinued as the deuterium atoms reach the surface of the tetrahedron.

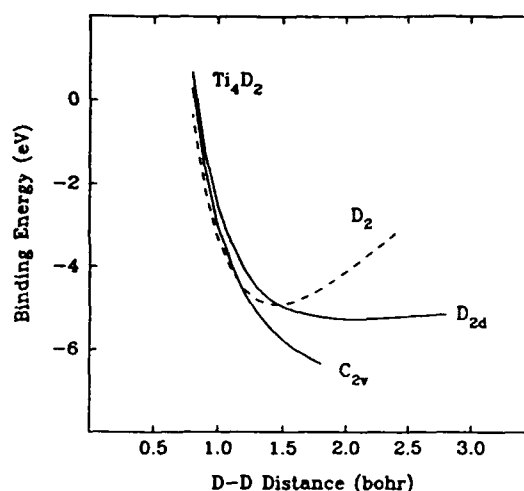


FIG. 4. Same as Fig. 3, but for titanium.

interstice of TiD_2 , although inside the TiD_2 octahedral interstice the D—D interaction is much more spherically symmetric, most likely because it is larger.

The preferred site for deuterium in titanium is the tetrahedral site. In TiD_2 all the tetrahedral sites are occupied by a single D atom and all octahedral sites are empty. The tetrahedral interstices for both metal hosts are smaller than the corresponding octahedral interstices. Therefore, if two deuterium atoms are placed inside the tetrahedral interstice of either metal at least one of them will be vigorously expelled. The lowest energy pathway for expulsion is through the center of one of the four faces of the tetrahedral interstice defined by three metal atoms. This can be seen from Figs. 3 and 4, in which two different paths for a pair of deuterium atoms to approach each other and to meet at the center are considered. In the first geometry the deuterium atoms lie symmetrically along the line passing through the center of the tetrahedron and connecting the center of opposite (not sharing a common vertex) Pd—Pd nearest-neighbor bonds. This cluster has D_{2d} symmetry. In the second geometry the two deuterium atoms lie along two different lines connecting the center of the tetrahedron and the center of a face. This cluster has C_{2v} symmetry. The binding-energy curves of two deuterium atoms along these two directions are compared with the binding-energy curve of free D_2 for palladium in Fig. 3, and for titanium in Fig. 4. For both hosts the lowest-energy D—D binding-energy curves are strongly repulsive at the boundaries of the tetrahedral interstices, the point at which the C_{2v} curves are discontinued.

V. LATTICE EXPANSION

The expansion of these lattices upon loading with deuterium has some effect on the D—D binding energy in these interstices. We can study that effect by recomputing the curves of Fig. 4 at the Ti—Ti nearest-neighbor distance appropriate to fcc TiD_2 instead of the distance appropriate to the empty bcc crystal. Figure 5 gives the metastable D_2 binding-energy curves, which have the

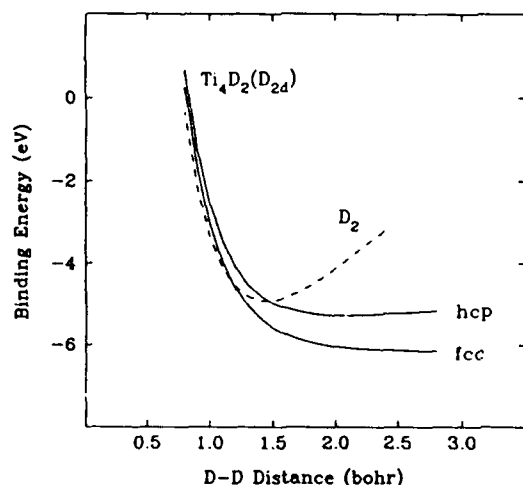


FIG. 5. LCGTO-LDF D-D metastable D_{2d} binding-energy curves in the Ti_4 tetrahedron. The upper solid curve is for Ti-Ti nearest-neighbor distances equal to the nearest-neighbor distance in hcp Ti. (This curve is identical to the corresponding curve of Fig. 4.) The lower solid curve is for the Ti-Ti distance expanded to that of fcc TiD_2 .

deuterium atoms on a line passing through opposite nearest-neighbor bonds of these two different sized tetrahedral interstices. Apart from the expanded fcc cluster having a slightly higher binding energy at larger D-D separations, there is a qualitative difference between these two curves. The curve corresponding to the smaller bcc cluster has a shallow minimum at 2.1 bohrs, while the curve for the expanded fcc cluster shows no minimum. Figure 6 gives the same comparison for the lower-energy D_2 binding-energy curves in the C_{2v} point-group symmetric Ti_4D_2 cluster. Both clusters vigorously

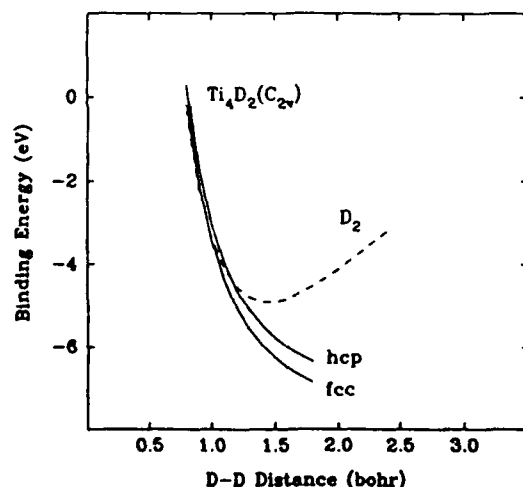


FIG. 6. LCGTO-LDF D-D C_{2v} binding-energy curves in the Ti_4 tetrahedron. The upper solid curve is for Ti-Ti nearest-neighbor distances equal to the nearest-neighbor distance in hcp Ti. (This curve is identical to the corresponding curve of Fig. 4.) The lower solid curve is for the Ti-Ti distance expanded to that of fcc TiD_2 .

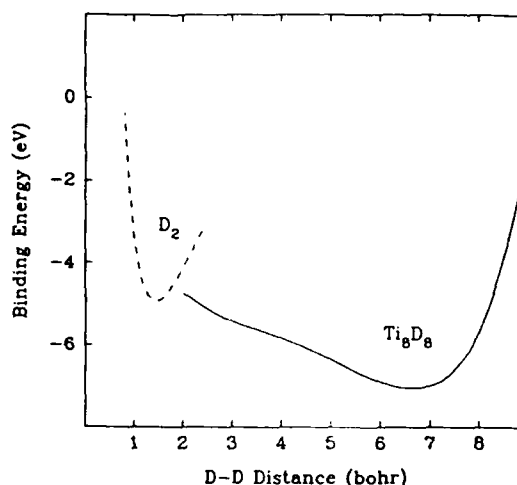


FIG. 7. LCGTO-LDF D-D binding-energy curve in the Ti_6D_2 cluster. This solid curve extends approximately the $\{111\}$ curve of Fig. 4 to larger distances.

expel the deuterium atoms through the center of adjacent faces of the tetrahedron.

Finally, in Fig. 7 we consider the effect of loading the titanium lattice with deuterium. We expand our D_{3d} point-group symmetric Ti_6D_2 cluster, which gave the $\{111\}$ curve of Fig. 2, to fcc dimensions and then add six more deuterium atoms and two more titanium atoms. The additional deuterium atoms are placed at six of the eight tetrahedral sites of the fcc crystal that are immediately outside the octahedron. The two empty tetrahedral sites are in the $\{111\}$ direction. The two additional titanium atoms are symmetrically placed at the first Ti lattice site encountered in the $\{111\}$ direction in the fcc TiD_2 crystal. The solid curve in this figure is the binding-energy curve of two deuterium atoms centrosymmetrically placed along the $\{111\}$ direction. The curve has a negative second derivative, but no maximum, when the two deuterium atoms are in the center of opposite faces of the octahedron at a separation of 4.8 bohrs. The minimum of the curve occurs at a separation of 6.6 bohrs. The two deuterium atoms occupy tetrahedral sites if they are separated by 7.3 bohrs.

For D-D distances where they overlap, this curve is about 1 eV higher in energy and has a steeper slope towards larger distances than the $\{111\}$ curve of Fig. 4. Because we found in Figs. 5 and 6 that expanding the lattice lowers the binding energy, we suspect that the dominant effect leading to this raising of the binding-energy curve is the fact that the cluster was loaded with deuterium. Thus loading the lattice with deuterium is more likely to increase the repulsive interaction between two deuterons that happen to be close together than to decrease that repulsive interaction.

VI. CONCLUSION

The effective interaction between deuterons in both interstices in both Pd and Ti is found to be more repulsive than in free molecular D_2 . Along directions of least

repulsion in all four interstices both deuterons repel each other out of the interstitial volume.

In this work, the above conclusion has been tested in three new ways. First, two different LDF's agree in predicting this repulsive interaction. Second, we have considered the fact that both lattices expand as they absorb deuterium. Expanding the titanium lattice gives more room for the deuterium atoms to push each other further apart. Third, loading the expanded lattice with spectator deuterium atoms also does not squeeze two deuterium atoms together. Combined with our earlier work that included empirical potentials and *ab initio* calculations, we

believe it unlikely that any theoretical approach to this problem would find a stable static configuration that could squeeze two deuterons even as close as they are in the free D_2 molecule.

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